

PUBCHEM_54605649

40730-78-7 | DTXSID90714109

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 1.47

Global applicability domain: Inside

Local applicability domain index: 3.53e-01

Confidence level: 5.42e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Picloram</div> <div>Measured: 1.30</div> <div>Predicted: 1.43</div>	<div>Image not found</div> <div>Asulam</div> <div>Measured: 1.60</div> <div>Predicted: 1.59</div>	<div>Image not found</div> <div>Cyromazine</div> <div>Measured: 2.30</div> <div>Predicted: 2.21</div>
<div>Image not found</div> <div>Monocrotophos</div> <div>Measured: 0.0</div> <div>Predicted: 4.41e-01</div>	<div>Image not found</div> <div>Endothal</div> <div>Measured: 2.09</div> <div>Predicted: 2.04</div>	